

# Orthogonal dimer-plaquette chain with alternating Ising-Heisenberg coupling

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We explore the dimer-plaquette Ising-Heisenberg chain, assembled between plaquette edge also known as orthogonal dimer plaquette. Using the local gauge symmetry of this model, we are able to map onto a simple spin-1 like Ising and spin-1/2 Heisenberg dimer model with single effective ion anisotropy, thereafter this model can be solved using the decoration transformation and transfer matrix approach. First we discuss the phase diagram at zero temperature of this model, where we find five ground states, one ferromagnetic, one antiferromagnetic, one triplet-triplet disordered and one triplet-singlet disordered phase, beside a dimer ferromagnetic-antiferromagnetic phase. It is interesting to note that, in the limit of pure Ising model there is a frustrated region. In addition, we discuss the thermodynamic properties such as entropy, where we display the residual entropy. The specific heat also is discussed, where we observe anomalous peaks close to the first order phase transition in the low temperature limit and for weak Heisenberg anisotropic coupling, but for strong Heisenberg anisotropic coupling, this anomalous peak disappear. Furthermore, using the nearest site correlation function it is possible also to analyze the pairwise thermal entanglement for both orthogonal dimers, as well as the we discuss the threshold temperature of the entangled region as a function of Hamiltonian parameters.

## I. INTRODUCTION

Quasi two-dimensional magnets have been attracted since 90 decades, such as the quasi-two-dimensional magnet  $\text{CaV}_4\text{O}_9$ [1], that has a layered structure where the magnetic  $\text{V}^{4+}$  ions have spin 1/2 and form a 1/5-depleted square lattice. As well as the polycrystalline  $\text{SrCu}_2(\text{BO}_3)_2$  having a two dimensional (2D) orthogonal network of Cu dimers, this cuprate, provides a 2D spin-gap system in which the ground state can be solved exactly[2, 3]. These quasi-two-dimensional systems are topologically equivalent to the theoretical model proposed by Shastri and Sutherland[4].

Motivated by the above real materials Ivanov and Richter[5] proposed the class of one-dimensional Heisenberg spin models (plaquette chains) related to the real materials[1–3], through numerical and analytical results was analyzed the zero temperature magnetic properties[5, 6]. While in reference [7] was discussed the sequence of first-order quantum phase transitions in a frustrated spin half dimer-plaquette chain. A detailed investigation about the first-order quantum phase transition of the orthogonal-dimer spin chain also was considered by Koga et al.[8], as well as the frustration-induced phase transitions in the spin- $S$  orthogonal-dimer chain[9].

A more recent investigation was developed by Ohanyan and Honecker[10], where they have been discussed the magnetothermal properties of the Ising-Heisenberg orthogonal-dimer chain with triangular XXZ clusters. Furthermore, in the last decade several quasi-one-dimensional Ising-Heisenberg model such as diamond chain were intensively investigated, mainly the thermodynamic properties and geometric frustration[11–14], magneto-caloric effect[15], as well as thermal entanglement[16, 17], among other physical quantities. Some other variant of the Ising-Heisenberg model also were considered, such as Ising-Hubbard model[18] and Hubbard model in the quasi-atomic limit[19] besides

spinless electrons[20] in diamond chain.

On the other hand, quantum entanglement is one of the most attractive types of correlations that can be shared only among quantum systems[21]. In recent years, many efforts have been devoted to characterizing qualitatively and quantitatively the entanglement properties of condensed matter systems, which are the natural candidate for application in quantum communication and quantum information. In this sense, it is quite relevant to study the entanglement of solid state systems such as spin chains[22]. The Heisenberg chain is one of the simplest quantum systems, which exhibits the entanglement, due to the Heisenberg interaction is not localized in the spin system. Several studies have been done on the threshold temperature for the pairwise thermal entanglement in the Heisenberg model with a finite number of qubits. Thermal entanglement of the isotropic Heisenberg chain has been studied in the absence [23] and in the presence of external magnetic field [24].

The outline of this work is as follows. In sec. 2 we present the dimer-plaquette Ising-Heisenberg chain; it is also discussed the zero temperature phase diagram. In sec. 3 we present the exact thermodynamic solution of the model, thus we discuss the entropy and specific heat. In sec. 4 we discuss the thermal entanglement and its threshold temperature. Finally in sec. 5, we summarize our results and draw our conclusions.

## II. ORTHOGONAL DIMER-PLAQUETTE ISING-HEISENBERG CHAIN

The theoretical investigation of the orthogonal dimer-plaquette models is motivated not only from the theoretical point of view, but also from the experimental viewpoint. It is worth to remark that the Heisenberg orthogonal dimer-plaquette model cannot be solved exactly at finite temperature. Motivated by the comments

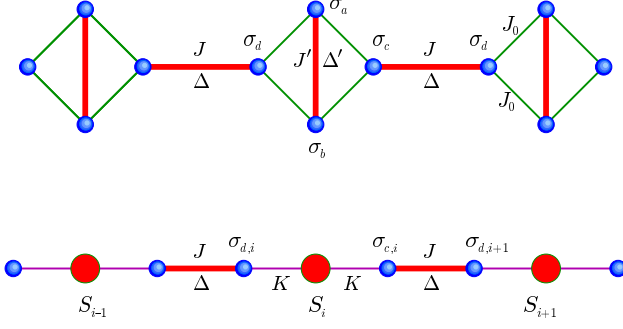


Figure 1: (Color online) Schematic representation of dimer-plaquette Ising-Heisenberg chain. (Above) Thick line corresponds to Heisenberg coupling, while the thin line corresponds to Ising coupling. (Below) Dimer plaquette mapping through local gauge symmetry.

given in the introduction, we consider the orthogonal-dimer plaquette chain with Ising-Heisenberg coupling as schematically described in figure 1. Therefore, the Hamiltonian for an orthogonal dimer-plaquette chain could be expressed by

$$H = - \sum_{i=1}^N \{ J'(\sigma_{a,i}, \sigma_{b,i})_{\Delta'} + J(\sigma_{c,i}, \sigma_{d,i})_{\Delta} + J_0(\sigma_{a,i}^z + \sigma_{b,i}^z)\sigma_{c,i}^z + (\sigma_{a,i+1}^z + \sigma_{b,i+1}^z)\sigma_{d,i}^z \}, \quad (1)$$

with

$$J'(\sigma_{a,i}, \sigma_{b,i})_{\Delta'} = J'(\sigma_{a,i}^x \sigma_{b,i}^x + \sigma_{a,i}^y \sigma_{b,i}^y) + \Delta' \sigma_{a,i}^z \sigma_{b,i}^z \quad (2)$$

where  $\sigma_{\gamma,i}^{\alpha}$  are the spin operators also known as Pauli matrices (with  $\alpha = \{x, y, z\}$ ) at plaquette  $i$  for particles  $\gamma = \{a, b, c, d\}$ , for detail see figure 1. The thick line correspond to Heisenberg coupling, while the thin line corresponds to Ising coupling. The Ising coupling parameter is denoted by  $J_0$ , whereas  $J$  ( $J'$ ) represents the  $x$  and  $y$  components of Heisenberg coupling and with  $\Delta$  ( $\Delta'$ ) we mean the anisotropic ( $z$ -component) coupling in the Heisenberg term for dimer  $ab$  and  $cd$  respectively.

To transform this model onto the well known mixed spin "Ising"-Heisenberg model, we use the following definition  $S_i^{\alpha} = \sigma_{a,i}^{\alpha} + \sigma_{b,i}^{\alpha}$ . By the use of  $S_i^{\alpha}$  definition we obtain the identity:  $(S_i^{\alpha})^2 = 2 + 2\sigma_{a,i}^{\alpha}\sigma_{b,i}^{\alpha}$ . Thereafter, we can easily establish the following transformation

$$J'(\sigma_{a,i}, \sigma_{b,i})_{\Delta'} = \frac{1}{2}S_i^2 + \frac{\Delta' - J'}{2}(S_i^z)^2 - (2J' + \Delta'), \quad (3)$$

and by  $S_i^2$  we just denote  $S_i^2 = S_i \cdot S_i$ , so, this matrix is given by

$$S_i^2 = 4 \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}, \quad (4)$$

rewritten the Hamiltonian in terms of operators  $S_i^z$  and  $S_i^2$  we have an Ising-Heisenberg chain model whose

Hamiltonian is given by  $H = H_0 + H'$ , with  $H_0 = (2J' + \Delta')N$ . Therefore, the transformed Hamiltonian reduce to

$$H' = - \sum \left\{ \frac{J'}{4}(S_i^2 + S_{i+1}^2) + \frac{\Delta' - J'}{4}[(S_i^z)^2 + (S_{i+1}^z)^2] + J(\sigma_{c,i}, \sigma_{d,i})_{\Delta} + J_0(S_i^z \sigma_{c,i}^z + \sigma_{d,i}^z S_{i+1}^z) \right\}. \quad (5)$$

We can observe from eq.(4) the matrix has a  $2 \times 2$  block matrix; hence, we can diagonalize this block matrix. It is interesting to note that the matrix  $S_i^z$  is still diagonal in the new basis, due to corresponding  $2 \times 2$  block matrix be null. Then, this means we can simultaneously diagonalize both matrices  $S_i^z$  and  $S_i^2$ . Recall those  $S_i^z$  and  $S_i^2$  are commutative operators. So, the diagonal matrices are expressed by

$$S_i^2 = \begin{bmatrix} 8 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8 \end{bmatrix} \quad \text{and} \quad S_i^z = \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{bmatrix}, \quad (6)$$

and whose corresponding eigenvector states are expressed as

$$|\tau_{+1}\rangle = |+\rangle, \quad (7)$$

$$|\tau_0\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle), \quad (8)$$

$$|s_0\rangle = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle), \quad (9)$$

$$|\tau_{-1}\rangle = |-\rangle. \quad (10)$$

The effective Ising "spin" in Hamiltonian (5) can be understood as a composition of one triplet state and one singlet state.

This transformation is possible because, the local gauge symmetry is only satisfied by Hamiltonian (1) when the Ising couplings  $ac$  ( $ad$ ) and  $bc$  ( $bd$ ) are identical.

### A. The zero temperature phase diagram

In order to analyze the phase diagram of the orthogonal-dimer plaquette, we assume the particular case  $J' = J$  and  $\Delta' = \Delta$ , following the parameter used in the literature[7–9].

The dimer-plaquette Ising-Heisenberg chain described by the Hamiltonian (1) exhibits five ground states. These states are expressed as

$$|FM\rangle = \prod_{i=1}^N |+\rangle_i \otimes |+\rangle_i, \quad (11)$$

$$|AFM\rangle = \prod_{i=1}^N |+\rangle_i \otimes |-\rangle_i, \quad (12)$$

One ferromagnetic (FM) phase and another antiferromagnetic (AFM) phase, with corresponding eigenvalues

given by

$$\begin{aligned} E_{FM} &= -2J' - 2\Delta' - \Delta - 4J_0, \\ E_{AFM} &= -2J' - 2\Delta' - \Delta + 4J_0. \end{aligned}$$

The other phase are composed by dimers in triplet-triplet (TT) phase and triplet-singlet (TS) phase,

$$|TT\rangle = \prod_{i=1}^N |\tau_0\rangle_i \otimes \frac{1}{\sqrt{2}} (|+-\rangle_i + |-+\rangle_i), \quad (13)$$

$$|TS\rangle = \prod_{i=1}^N |\tau_0\rangle_i \otimes \frac{1}{\sqrt{2}} (|+-\rangle_i - |-+\rangle_i), \quad (14)$$

where the corresponding eigenvalues become

$$\begin{aligned} E_{TT} &= \Delta - 2J - 4J', \\ E_{TS} &= \Delta + 2J. \end{aligned}$$

It is worthy to mention that the state given by eqs.(13) and (14) becomes frustrated state only when  $J = 0$  (Ising limit).

Finally, the dimer-antiferromagnetic (DFA) state can be expressed by

$$|DFA\rangle = \prod_{i=1}^{N/2} |+\rangle_i^+ \otimes |\eta_{2,-2}\rangle_i \otimes |-\rangle_i \otimes |\eta_{2,-2}\rangle, \quad (15)$$

with

$$|\eta_{2,-2}\rangle = \frac{(|+-\rangle_i + \vartheta|-+\rangle_i)}{\sqrt{1+\vartheta^2}}, \quad (16)$$

and

$$\vartheta = \frac{\sqrt{4J_0^2 + J^2} + 2J_0}{J}. \quad (17)$$

Hereafter the corresponding dimer-antiferromagnetic eigenvalue becomes

$$E_{DFA} = -2J' - 2\Delta' + \Delta - 2\sqrt{4J_0^2 + J^2}.$$

In order to display the phase diagram at zero temperature, we plot  $J$  versus  $\Delta$ , assuming fixed value for  $J_0 = 1(-1)$  FM(AFM) respectively. As shown in figure 2(a). For  $\Delta < -2$ , there is a boundary between TS and TT state at  $J = 0$ , whereas for  $-2 \leq \Delta \leq 0.5$  the state TS (TT) is limited by DFA region whose boundary is given by  $\Delta = 2|J| - \sqrt{4 + J^2}$ , when  $J > 0$  ( $J < 0$ ) respectively. While for  $\Delta \geq 0.5$  the states TS (TT) is limited by FM(AFM) region  $\Delta = |J| - 1$ . Furthermore, the boundary between DFA and FM(AFM) region is represented by the curve  $\Delta = \sqrt{4 + J^2} - 2$ .

While in figure 2(b), we observe the phase diagram from another viewpoint,  $\Delta$  against  $J_0$ , assuming fixed  $J = 1$ . In this picture the TS and TT phase is displayed in same region, while AFM and FM states are illustrated

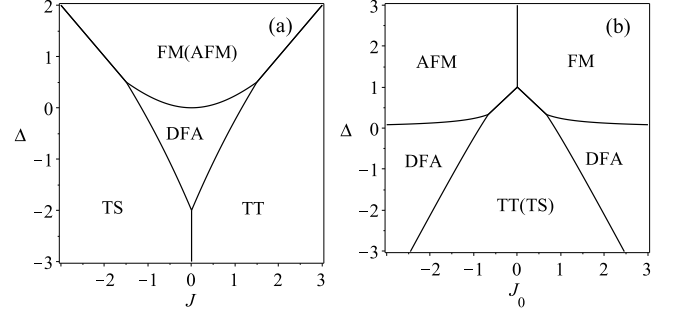


Figure 2: (a) Phase diagram at zero temperature as a dependency of  $J$  and  $\Delta$  for a fixed value of  $J_0 = 1$ . (b) Phase diagram at zero temperature as a dependency of  $J_0$  and  $\Delta$  for a fixed value of  $J = 1$ .

for  $J_0 > 0$  ( $J_0 < 0$ ) respectively. The boundary between FM(AFM) and TT(TS) is given by  $\Delta = 1 - |J_0|$  for  $|J_0| < 2/3$ . Whereas the DFA region appears for  $|J_0| > 2/3$ , which is limited by TT(TS) region and this boundary curve becomes  $\Delta = 2 - \sqrt{4J_0^2 + 1}$ , and finally the boundary between FM(AFM) region is described by the curve  $\Delta = \sqrt{4J_0^2 + 1} - 2|J_0|$ .

### III. THE THERMODYNAMICS OF THE MODEL

The method to be used will be the decoration transformation proposed in early 50 decade by Syozi [25] and Fisher [26]. Afterward this approach was the subject of study in reference [27], for the case of multi-spins. Similar generalization was developed by Strečka [28] for the hybrid system (e.g. Ising-Heisenberg). Another interesting variant of this approach also was discussed previously, where was proposed a direct transformation instead of several step by step transformation [29]. Consequently, the decoration transformation approach is widely used to solve spins models, besides, the decoration transformation approach can also be applied to electron coupling system such has been applied for the case of spinless fermion on diamond structure[20], and as well as for Hubbard model in the quasi-atomic limit[19].

In order to study the thermodynamics of the dimer-plaquette Ising-Heisenberg chain, we will use the decoration transformation proposed in reference [29] together with the usual transfer matrix technique [30]. So, let us start considering the partition function as follow

$$\mathcal{Z}_N = e^{-\beta H_0} \text{tr} \left( \prod_{i=1}^N e^{-\beta H'} \right), \quad (18)$$

where  $\beta = 1/kT$ , with  $k$  being the Boltzmann constant and  $T$  is the absolute temperature, and assuming  $H'$  is given by eq.(5).

The effective model can be solved by the usual transfer matrix approach[30]. Inasmuch as the transfer matrix of

the Hamiltonian (5) is reduced to

$$\mathbf{T} = \begin{bmatrix} w_{1,1} & w_{1,0}x'^2 & w_{1,0} & w_{1,-1} \\ w_{1,0}x'^2 & w_{0,0}x'^4 & w_{0,0}x'^2 & w_{1,0}x'^2 \\ w_{1,0} & w_{0,0}x'^2 & w_{0,0} & w_{1,0} \\ w_{1,-1} & w_{1,0}x'^2 & w_{1,0} & w_{1,1} \end{bmatrix}, \quad (19)$$

with

$$w_{1,1} = x'^2 z'^2 [z(y^4 + y^{-4}) + z^{-1}(x^2 + x^{-2})], \quad (20)$$

$$w_{1,0} = x' z' [z(y^2 + y^{-2}) + z^{-1}(x_1^2 + x_1^{-2})], \quad (21)$$

$$w_{1,-1} = x'^2 z'^2 [2z + z^{-1}(x_2^2 + x_2^{-2})], \quad (22)$$

$$w_{0,0} = 2z + z^{-1}(x^2 + x^{-2}), \quad (23)$$

where we have introduced the following notations  $x = e^{\beta J}$ ,  $z = e^{\beta \Delta}$ ,  $x' = e^{\beta J'}$ ,  $z' = e^{\beta \Delta'}$  and  $y = e^{\beta J_0}$ . Furthermore, we define also the following exponentials  $x_1 = e^{\beta \sqrt{J^2 + J_0^2}}$  and  $x_2 = e^{\beta \sqrt{J^2 + 4J_0^2}}$ .

In order to diagonalize the transfer matrix  $\mathbf{T}$ , we perform the determinant of the transfer matrix, which is expressed as follow

$$\lambda(\lambda^2 - a_1\lambda + a_0)(\lambda - w_{1,1} + w_{1,-1}) = 0, \quad (24)$$

here, the coefficients of the quadratic term eq.(24) is given by

$$a_1 = w_{1,1} + w_{0,0}(1 + x'^4) + w_{1,-1}, \quad (25)$$

$$a_0 = (1 + x'^4) [w_{0,0}(w_{1,1} + w_{1,-1}) - 2w_{1,0}^2],$$

Therefore, the eigenvalues can be expressed as

$$\lambda_0 = \frac{1}{2} \left( a_1 + \sqrt{a_1^2 - 4a_0} \right), \quad (26)$$

$$\lambda_1 = \frac{1}{2} \left( a_1 - \sqrt{a_1^2 - 4a_0} \right), \quad (27)$$

$$\lambda_2 = x'^2 z'^2 \left[ z(y^2 - y^{-2})^2 + \frac{(x^2 + x^{-2} - x_2^2 - x_2^{-2})}{z} \right], \quad (28)$$

$$\lambda_3 = 0. \quad (29)$$

In the thermodynamic limit, the free energy per unit cell is given only by the largest eigenvalue of transfer matrix, and for our case, we can easily verify the first eigenvalues  $\lambda_0$  become always the largest one. Thus, the free energy can be expressed by the relation below

$$f = 2J' + \Delta' - \frac{1}{\beta} \ln(\lambda_0). \quad (30)$$

The first term of the free energy is a trivial constant energy, obtained during the local gauge transformation, which is irrelevant for thermodynamis quantities. Note that the free energy is valid for arbitrary value of  $J'$  and  $\Delta'$ , although here we consider only a particular case  $J' = J$  and  $\Delta' = \Delta$ , following the parameter used in the literature[7–9]. Therefore, any additional properties can be obtained straightforwardly from eq.(30).

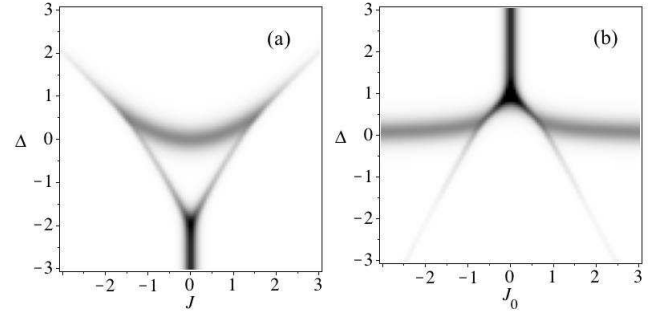


Figure 3: Density plot of entropy, darkest region corresponds to higher entropy. (a) Entropy as a dependency of  $J$  and  $\Delta$  for a fixed value of  $J_0 = 1$ . (b) Entropy as a dependency of  $J_0$  and  $\Delta$  for a fixed value of  $J = 1$ .

### A. Entropy and specific heath

In order to accomplish with our discussion concerning to the thermodynamics properties, let us illustrate the entropy ( $S = -\partial f / \partial T$ ) in fig. 3(a) for the low temperature limit as a function of  $\Delta$  and  $J$ , whereas, in fig.3(b) the entropy is illustrated as a function of  $\Delta$  and  $J_0$ . Dark region corresponds to higher entropy, while the white region corresponds to zero entropy. However, as soon as the temperature decreases the entropy leads to zero, unless, for  $J = 0$  and  $\Delta \leq -2$  (pure Ising chain) the dark line will remain when temperature decreases, leading to a residual entropy  $S_0 = 2 \ln(2)$ , that illustrates the geometric frustration region of orthogonal plaquette Ising chain.

Finally, we discuss also another interesting thermodynamic quantity called the specific heat ( $C = -T \partial^2 f / \partial T^2$ ). In figure 4, we plot the specific heat as a function of the temperature  $T$  for a fixed coupling parameter  $J_0 = 1.0$  and a fixed value of  $J = 1.0$ . By a solid line is represented the specific heat curve when  $\Delta = 0, 0.5$  and  $1.0$ , while, for dashed line we illustrate the specific heat for  $\Delta = -0.5$ , and  $-1.0$ . For anisotropic parameter  $\Delta = \pm 0.5$  and  $0$ , the plot illustrates a small anomalous peak due to the zero temperature phase transition influence, although for  $\Delta = \pm 1.0$  this anomalous peak disappear.

### B. Pair correlation function

The nearest site correlation function between dimers can be obtained using a derivative of the free energy given by eq.(30). Then, in order to perform the derivative of free energy, we need to assume the parameter  $J'$  and  $J$  as independent parameter, similarly  $\Delta'$  and  $\Delta$  also are considered as independent parameters. Despite for physical quantities, the term  $2J' + \Delta'$  in the free energy be irrelevant, this term cannot be neglected when we calculate

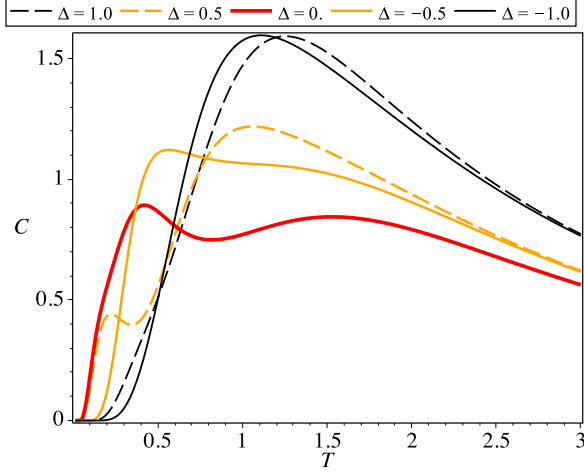


Figure 4: (Color online) Specific heat as a temperature dependency, for several values of anisotropic parameter.

the correlation function as expressed below:

$$\langle \sigma_a^x \sigma_b^x \rangle = -\frac{1}{2} \frac{\partial f}{\partial J'} = -1 + \frac{x'}{2\lambda_0} \frac{\partial \lambda_0}{\partial x'}, \quad (31)$$

$$\langle \sigma_a^z \sigma_b^z \rangle = -\frac{\partial f}{\partial \Delta'} = -1 + \frac{z'}{\lambda_0} \frac{\partial \lambda_0}{\partial z'}, \quad (32)$$

$$\langle \sigma_c^x \sigma_d^x \rangle = -\frac{1}{2} \frac{\partial f}{\partial J} = \frac{x}{2\lambda_0} \frac{\partial \lambda_0}{\partial x}, \quad (33)$$

$$\langle \sigma_c^z \sigma_d^z \rangle = -\frac{\partial f}{\partial \Delta} = \frac{z}{\lambda_0} \frac{\partial \lambda_0}{\partial z}. \quad (34)$$

Here, we present the relation of the correlation function in terms of the largest eigenvalue of the transfer matrix  $\lambda_0$ .

#### IV. THERMAL ENTANGLEMENT

Another interesting property we consider in this work, will be the quantum entanglement of the Ising-Heisenberg orthogonal dimer plaquette model. As a measure of entanglement for two arbitrary mixed states of dimers, we use the quantity called concurrence[31], which is defined in terms of reduced density matrix  $\rho$  of two mixed states

$$\mathcal{C}(\rho) = \max\{0, 2\Lambda_{max} - \text{tr}\sqrt{R}\}, \quad (35)$$

assuming

$$R = \rho \sigma^y \otimes \sigma^y \rho^* \sigma^y \otimes \sigma^y, \quad (36)$$

where  $\Lambda_{max}$  is the largest eigenvalue of the matrix  $\sqrt{R}$  and  $\rho^*$  represent the complex conjugate of matrix  $\rho$ , with  $\sigma^y$  being the Pauli matrix.

For the case of infinite chain, the reduced density operator elements[32] could be expressed in terms of the

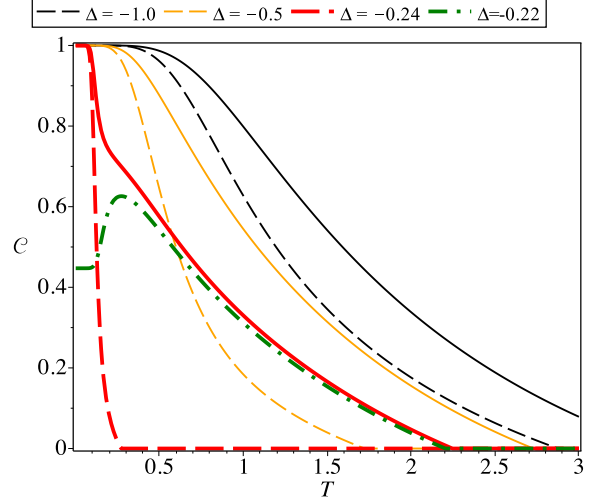


Figure 5: (Color online) Concurrence for several values of anisotropic parameter as a function of  $T$ . Dashed line corresponds for  $ab$ -dimer while the solid line represents  $cd$ -dimer.

correlation function between two entangled particles[33], consequently the concurrence between  $ab$ -dimer becomes

$$\mathcal{C}_{ab} = \max\{0, |\langle \sigma_a^x \sigma_b^x \rangle| - \frac{1}{2}|1 + \langle \sigma_a^z \sigma_b^z \rangle|\}, \quad (37)$$

similarly the concurrence between  $cd$ -dimer reads

$$\mathcal{C}_{cd} = \max\{0, |\langle \sigma_c^x \sigma_d^x \rangle| - \frac{1}{2}|1 + \langle \sigma_c^z \sigma_d^z \rangle|\}. \quad (38)$$

Surely, we can obtain also equivalent result using the approach described in reference [16].

It is worthy to mention that the zero temperature entanglement for  $ab$ -dimer is maximally entangled in TS and TT region  $\mathcal{C}_{ab} = 1$ , while, in all other region the  $ab$ -dimer becomes unentangled ( $\mathcal{C}_{ab} = 0$ ). Whereas the  $cd$ -dimer also is maximally entangled in same (TS and TT) region  $\mathcal{C}_{cd} = 1$ ; furthermore the DFA region now also becomes an entangled region whose concurrence is given by  $\mathcal{C}_{cd} = \frac{|J|}{\sqrt{4J_0^2 + J^2}}$  and it depends of  $J$  and  $J_0$ . It is worth to notice, when  $J = 0$  this region becomes unentangled, which is perfectly coherent since the model reduces to orthogonal plaquette Ising chain. Another special possibility is when  $J_0 = 0$ , the orthogonal dimer plaquette reduces simply to independent entangled dimers. While the FM and AFM region are unentangled  $\mathcal{C}_{cd} = 0$ .

In figure 5 is plotted the concurrence  $\mathcal{C}$  as a function of the temperature: for  $\Delta = -1$  the dashed and solid line corresponds to  $ab$ -dimer and  $cd$ -dimer respectively. However, the  $ab$ -dimer entanglement vanishes for  $T \approx 2.9$  while, for  $cd$ -dimer the entanglement vanishes at  $T \approx 4.0$ . For weaker anisotropic coupling ( $\Delta$ ) this difference becomes more significantly, say i.e. for  $\Delta = -0.24$ , the  $cd$ -dimer (solid line) entanglement vanishes for  $T \approx 2.25$ , whilst for  $ab$ -dimer the entanglement vanishes at  $T \approx 0.28$  (dashed line). For a bit weaker

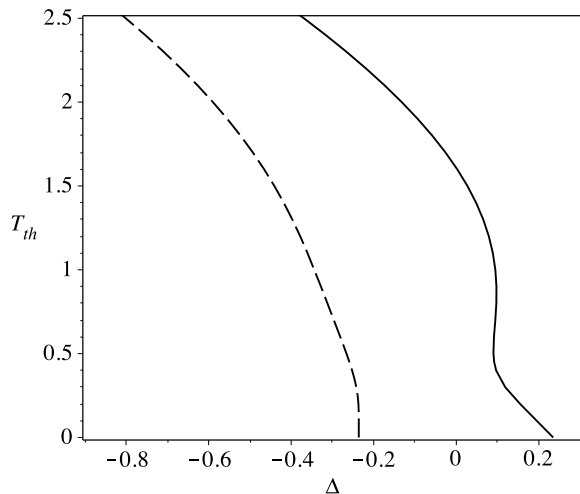


Figure 6: Threshold temperature  $T_{th}$  as a function of  $\Delta$ , for fixed  $J_0 = 1$  and  $J = 1$ . Dashed line corresponds for  $ab$ -dimer, while the solid line represents  $cd$ -dimer.

anisotropic parameter  $\Delta = -0.22$ , the  $ab$ -dimer becomes untangled region for any temperature, while  $cd$ -dimer entanglement vanishes at  $T \approx 2.24$ .

### A. Threshold temperature

The threshold temperature can be obtain when  $ab$ -dimer concurrence becomes null ( $|\langle \sigma_a^x \sigma_b^x \rangle| = \frac{1}{2}|1 + \langle \sigma_a^z \sigma_b^z \rangle|$ ), and similarly for  $cd$ -dimer, the concurrence will become null when ( $|\langle \sigma_c^x \sigma_d^x \rangle| = \frac{1}{2}|1 + \langle \sigma_c^z \sigma_d^z \rangle|$ ).

The threshold temperature is illustrated in figure 6 as a function of anisotropic parameter for fixed values of  $J_0 = 1$  and  $J = 1$ . The dashed line correspond for the  $ab$ -dimer threshold temperature, and in the low temperature limit, the threshold temperature leads to  $T_{th} = 2 - \sqrt{5}$ . Whereas the solid line represents the  $cd$ -dimer threshold temperature; in the low temperature limit it leads to  $T_{th} = \sqrt{5} - 2$ . It is worthy to highlight that the threshold temperature for  $cd$ -dimer exhibits a small reentrance around to  $\Delta = 0.1$ .

Another way to display the entanglement phase diagram is in units of threshold temperature as displayed in figure 7, the boundary between entangled region and untangled region is given by a solid (red) line. The black region correspond to maximally entangled region, and white region corresponds to untangled region, while light gray region corresponds to weak concurrence similarly dark gray corresponds to strong concurrence. The entangled phase diagram  $J$  against  $\Delta$  in units of  $T_{th}$ , behaves quite similar for both  $ab$ -dimer and  $cd$ -dimer, although, for  $ab$ -dimer the untangled region appears already significantly for  $\Delta \geq -3$  and small values of  $J$ , while for  $cd$ -dimer the untangled region becomes relevant only for  $\Delta \geq -1$  and small values of  $J$ . Certainly this is in agreement with the zero temperature phase diagram displayed

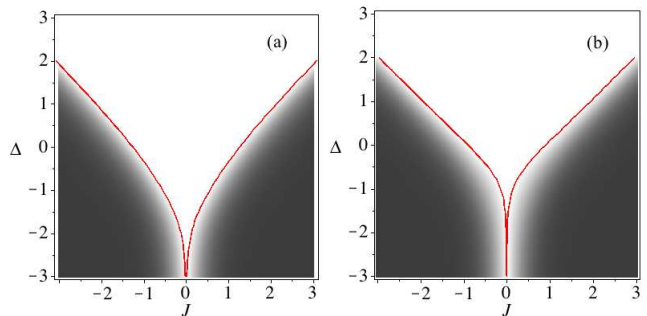


Figure 7: (Color online) Density plot of concurrence in units of  $T_{th}$ , darkest region corresponds to higher entanglement. (a) Concurrence for  $ab$ -dimer as a dependency of  $J$  and  $\Delta$  for a fixed value of  $J_0 = 1$ . (b) Concurrence for  $cd$ -dimer as a dependency of  $J$  and  $\Delta$  for a fixed value of  $J_0 = 1$ .

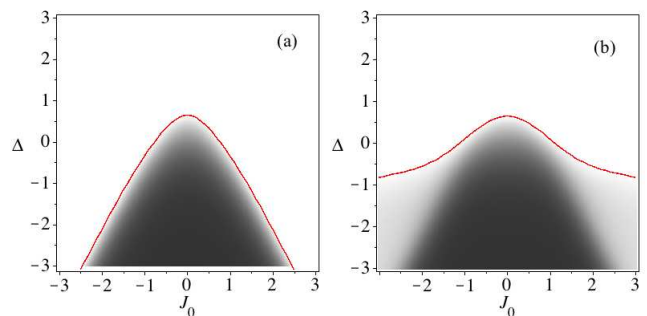


Figure 8: Density plot of Concurrence in units of  $T_{th}$ , darkest region corresponds to higher entanglement. (a) Concurrence for  $ab$ -dimer as a dependency of  $J_0$  and  $\Delta$  for a fixed value of  $J = 1$ . (b) Concurrence for  $cd$ -dimer as a dependency of  $J_0$  and  $\Delta$  for a fixed value of  $J = 1$ .

in figure 2(a).

Additional density plot of entangled phase diagram is displayed in figure 8 in terms of  $\Delta$  and  $J_0$ , once again in units of  $T_{th}$ , the phase diagrams for  $ab$ -dimer is given in fig.2(a), and the phase diagram for  $cd$ -dimer is illustrated in fig.2(b). Here, we observe the phase diagram between  $ab$ -dimer and  $cd$ -dimer are quite different, but still are closely related to the zero temperature phase diagram illustrated in figure 2(b). Although the darkest (strongly entangled) region are very similar for both dimers.

## V. CONCLUSION

In this work, we studied the dimer-plaquette Ising-Heisenberg chain, assembled between plaquette edge also known as orthogonal dimer plaquette[5–10]. Using the local gauge symmetry of this model, we are able to map onto a simple spin-1 like Ising and spin 1/2 Heisenberg dimer model with single effective ion anisotropy. Thereafter, this model can be solved using the decoration transformation[25–27, 29] and transfer matrix approach. First we discuss the phase diagram at zero tem-

perature of this model, where we found five ground states as illustrated in figure 2, one ferromagnetic, one anti-ferromagnetic, one tripled-triplet disordered and triplet-singlet disordered phase, beside a dimer ferromagnetic-antiferromagnetic phase. It is interesting to remark that, in the limit of pure Ising model this exhibits a frustrated region. Furthermore, are discussed the thermodynamic properties such as entropy, specific heat as well as the correlation function. For the specific heat curve we observe an anomalous peaks close to the first order phase transition in the low temperature limit (fig.4), for weak Heisenberg anisotropic coupling, but for strong Heisenberg anisotropic coupling, this anomalous peak disappear. Additionally, using the nearest site correlation function it is possible to analyze the pairwise thermal entanglement for both *ab*-dimer and *cd*-dimer, as well as the threshold temperature of the entangled region are discussed as a function of the Hamiltonian parameters.

There is some significant difference between both dimers (*ab*-dimers and *cd*-dimers) which is in agreement in the low temperature limit. However, for strong entanglement, both dimers are quite similar. As a consequence of this difference, we can illustrate one interesting result, regarding to the reentrance type of threshold temperature for *cd*-dimer, despite for *ab*-dimer there is no reentrance temperature.

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